

Stationary localized states due to quadratic nonlinearity in one dimensional systems

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Abstract

We investigate the effect of a nondegenerate quadratic nonlinear dimeric impurity on the formation of stationary localized states in one dimensional systems. We also consider the formation of stationary localized states in a fully nonlinear system where alternative sites have same nonlinear strengths. Appropriate ansatzs have been chosen for all the cases which reproduce known results for special cases. Connection of the stability of a state with its energy is presented graphically.

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I. INTRODUCTION

The discrete nonlinear Schrödinger equation which describes a number of phenomena in condensed matter physics, non-linear optics and other fields of physics [1-6] may be generally written as

$$i\frac{dC_m}{dt} = -\chi_m f_m(|C_m|)C_m + V_{m,m+1}C_{m+1} + V_{m,m-1}C_{m-1}$$

where $V_{m,m+1} = V_{m+1,m}^*$; and $m = 1, 2, 3, \dots, n$. (1)

In eq.(1) χ_m is the nonlinearity parameter associated with m -th grid point and $V_{m,m+1}$ is the nearest neighbor hopping matrix element . Since, $\sum_m |C_m|^2$ is made unity by choosing appropriate initial conditions, $|C_m|^2$ can be interpreted as the probability of finding a particle at the m -th grid point. The nonlinearity term $f_m(|C_m|)$ arises due to the coupling of the vibration of masses at the lattice points to the motion of a quasi-particle in the high frequency lattice vibration limit [3]. The DNLSE in other physical context is known as the discrete self trapping equation (DST). A number of works on the DNLSE and the DST have been reported [7-10].

As for the application of the DNLSE particularly in condensed matter physics, we cite among others the exciton propagation in Holstein molecular crystal chain [2]. In general, the exciton propagation in quasi one dimensional systems [11] having short range electron phonon interaction can be adequately modeled by the DNLSE. Other examples include non-linear optical responses in superlattices formed by dielectric or magnetic slabs [12] and the mean field theory of a periodic array of twinning planes in the high T_c superconductors [13]. We also note that the vibration in the nonlinear Klein-Gordon chain in certain restrictive conditions can be described by the DNLSE [14].

One important feature of the DNLSE is that this can yield stationary localized (SL) states. These SL states might play a relevant role in the nonlinear DNA dynamics [15] and also in the energy localization in nonlinear lattices [16]. It has been shown that the presence of a nonlinear impurity can produce SL states in one, two and three dimension [17-24]. The

formation of SL states due to the presence of a single and a degenerate dimeric nonlinear impurity in a few linear hosts has been studied in details [20]. The same problem is also studied starting from an appropriate Hamiltonian [23]. The fixed point of the Hamiltonian [21-24] which generates the appropriate DNLSE can also produce the correct equations governing the formation of SL states. We further note that the appropriate ansatz for the dimer problem has been obtained in our earlier analysis [20]. Furthermore, the formation of intersite peaked and dipped stationary localized states has been studied using the dimeric ansatz [24]. The formation of SL states in a perfect nonlinear chain containing one nonlinear impurity as well as a degenerate nonlinear dimeric impurity has been studied [24]. In another study the formation of SL states in a perfect nonlinear Cayley tree and in a linear Cayley tree with dimeric impurity has been considered.

So far degenerate nonlinear dimer impurity has been considered . Naturally question arises what happens if the impurities in the dimer are nondegenerate . We therefore plan to study the effect of nondegeneracy in impurities on the formation of SL states. Three linear hosts are studied, namely, a perfect one dimensional chain , a Cayley tree and a linear chain with a bond defect . We also consider the formation of SL states in a fully nonlinear chain having a regular binary alloy composition. Appropriate ansatzs have been fitted in all the cases to obtain the results.

The organization of the paper is as follows. In sec. II we consider the effect of nonlinear nondegenerate dimer on the formation of SL states in linear systems. Sec. III deals with the formation of SL states in a fully nonlinear system and the stability analysis of the SL states. Finally we summarize our findings in Sec. IV.

II. NONDEGENERATE NONLINEAR DIMER IMPURITY

We consider a system of one dimensional chain consisting of a nondegenerate nonlinear dimer impurity of the kind $\chi|C|^\sigma$ (power law impurity) where σ is arbitrary. The dimeric impurity is placed at sites 0 and 1 of the chain. The dimer is nondegenerate in the sense

that nonlinear strengths at sites 0 and 1 are different and denoted by χ_0 and χ_1 . Therefore, the relevant Hamiltonian for this system is

$$H = \frac{1}{2} \sum_{m=-\infty}^{\infty} [C_m C_{m+1}^* + h.c.] + \frac{V-1}{2} [C_0 C_1^* + h.c.] + \frac{\chi_0}{\sigma+2} |C_0|^{\sigma+2} + \frac{\chi_1}{\sigma+2} |C_1|^{\sigma+2}. \quad (2)$$

Hopping matrix element between sites 0 and 1 is V and others are taken to be unity. The Hamiltonian with $V = 1$ describes a perfect chain, $V < 1$ describes a system of perfect Cayley tree while $V > 1$ describes 1-dimensional chain with a bond defect between sites 0 and 1. Furthermore, all the systems contain a nondegenerate nonlinear dimeric impurity spanning the zeroth and first sites. In case of the Cayley tree V takes the form of $\frac{1}{\sqrt{K}}$, where K stands for the connectivity of the Cayley tree. The relevant transformation of the Cayley tree into an effective 1-dimensional system has been already presented [24]. Since we are interested in the possible solutions for SL states due to the presence of dimeric impurity we assume

$$C_m = \phi_m e^{-iEt} \quad (3)$$

The presence of a dimeric impurity in the system suggests us to consider the following form of ϕ_m

$$\begin{aligned} \phi_m &= [Sgn(E)\eta]^{m-1} \phi_1 & m \geq 1 \\ \phi_{-|m|} &= [Sgn(E)\eta]^{|m|} \phi_0 & m \leq 0 \end{aligned} \quad (4)$$

We further note that the above form of ϕ_m can be derived from Green's function analysis [20]. Here $\eta \in [0, 1]$ is given by $\eta = \frac{1}{2}[|E| - \sqrt{E^2 - 4}]$. We further define $\beta = \phi_0/\phi_1 \in [-1, 1]$. Now normalization condition, $\sum_{m=-\infty}^{\infty} |C_m|^2 = 1$ together with eqs.(3) and (4) give

$$|\phi_0|^2 = \frac{1 - \eta^2}{1 + \beta^2} \quad (5)$$

Using eqs.(3), (4) and (5) in the Hamiltonian H , we obtain the effective Hamiltonian of the reduced dynamical system given by

$$H_{eff} = Sgn(E)\eta + V\beta \frac{1 - \eta^2}{1 + \beta^2} + \frac{1}{\sigma+2} \left(\frac{1 - \eta^2}{1 + \beta^2} \right)^{\frac{\sigma+2}{2}} (\chi(1 + |\beta|^{\sigma+2}) + \delta(1 - |\beta|^{\sigma+2})) \quad (6)$$

Here we have defined χ and δ as $\chi = (\chi_0 + \chi_1)/2$ and $\delta = (\chi_0 - \chi_1)/2$. The Hamiltonian consists of two variables namely β and η . SL states can be obtained from the fixed point solutions [21-23] of the Hamiltonian, H_{eff} , of the reduced dynamical system. The fixed point solutions satisfy equations $\partial H_{eff}/\partial\beta = 0$ and $\partial H_{eff}/\partial\eta = 0$.

Equation $\partial H_{eff}/\partial\beta = 0$ gives

$$[1 - \eta]^{\frac{\sigma}{2}} = \frac{V(1 - \beta^2)(1 + \beta^2)^{\frac{\sigma}{2}}}{\beta[(\chi + \delta) - |\beta|^\sigma(\chi - \delta)]}. \quad (7)$$

Equation $\partial H_{eff}/\partial\eta = 0$ gives

$$\eta = \frac{Sgn(E)\beta[(\chi + \delta) - |\beta|^\sigma(\chi - \delta)]}{V[(\chi + \delta) - |\beta|^{\sigma+2}(\chi - \delta)]}. \quad (8)$$

For fixed values of χ and δ number of solutions satisfying eqs.(7) and (8) simultaneously will give the number of possible SL states. This can be obtained for arbitrary σ but we will consider $\sigma = 0$ and $\sigma = 2$. The reason behind taking $\sigma = 0$ case is that the result is already known and hence the appropriateness of the ansatz can be verified. $\sigma = 2$ is considered because it is physically more relevant.

1. $\sigma = 0$

For $\sigma = 0$, the system reduces to a perfectly linear 1-dimensional chain with two static impurities χ_0 and χ_1 at sites 0 and 1 respectively. In this case eq.(7) directly gives

$$\beta_\pm = -\frac{\delta}{V} \pm \sqrt{\frac{\delta^2}{V^2} + 1}. \quad (9)$$

In passing we note that , when $\delta = 0$ i.e. the dimer impurity becomes linear and degenerate, $\beta = \pm 1$ are only permissible solutions. This is consistent with our earlier work [20]. On the other hand $\delta \neq 0$ necessitates $\beta \neq \pm 1$ for permissible solutions. Substituting eq.(9) in eq.(8) we obtain

$$\frac{1}{\chi} = \frac{\eta}{Sgn(E) \mp \eta\sqrt{\delta^2 + V^2}}. \quad (10)$$

Eq.(10) along with signature of E gives four expressions for $1/\chi$. From each expression we will get a critical line in the (χ, δ) plane. The critical lines can be obtained by putting $\eta = 1$ in eq.(10). The equations describing the critical lines are

$$\begin{aligned}
\chi_c^{(1)} &= 1 + \sqrt{\delta^2 + V^2} \\
\chi_c^{(2)} &= -1 - \sqrt{\delta^2 + V^2} \\
\chi_c^{(3)} &= 1 - \sqrt{\delta^2 + V^2} \\
\chi_c^{(4)} &= -1 + \sqrt{\delta^2 + V^2}.
\end{aligned} \tag{11}$$

These critical lines are shown in fig.(1) for $V = 1$, in fig.(2) for $V = 0.5$ (which corresponds to a Cayley tree with $K = 4$) and in fig.(3) for $V = \sqrt{2}$. There are several regions in the (χ, δ) plane bounded by the critical lines in all the figures. There are regions containing no SL state, one SL state appearing above the host band, one SL state appearing below the band, two SL states with one below and one above the band and two SL states appearing above as well as below the band. Since our results for $V = 1$ and $V = 0.5$ agree with known results [25], the validity of our starting ansatz is established.

2. $\sigma = 2$

We now investigate the case where nonlinearity power $\sigma = 2$. Physically $\sigma = 2$ can appear when the masses at the lattice points are treated as Einstein oscillators. From eq.(7) we again note that for $\delta = 0$, $\beta = \pm 1$ are permissible solutions. On the other hand, for $\delta \neq 0$, $\beta = \pm 1$ are not permissible solutions. From eqs.(7) and (8) we obtain the relevant equation for SL states. The equation is given as

$$\frac{1}{\chi} = \frac{\beta[(1+\alpha) - (1-\alpha)\beta^2][V^2[(1+\alpha) - (1-\alpha)\beta^4]^2 - \beta^2[(1+\alpha) - (1-\alpha)\beta^2]^2]}{V^3[1 - \beta^4][(1+\alpha) - (1-\alpha)\beta^4]^2} \tag{12}$$

where $\alpha = \delta/\chi$. Using eq.(12) we have obtained the full phase diagram of SL states in (χ, δ) plane for $V = 1$ and this is shown in fig.(4). There are various regions in the phase diagram numbered according to number of possible SL states in the region. Along the $\delta = 0$ line, we note that for $\chi \geq 0$, there are three critical values of χ , namely, 1, $8/3$ and 8. These critical values are in agreement with the values obtained in our earlier work [23]. In this case, maximum number of SL states appearing is five. With the use of same eq.(12), we have also obtained the phase diagram for SL states in (χ, δ) plane for a Cayley tree with connectivity $K = 4$ ($V = 0.5$). This is shown in fig.(5). Maximum number of possible SL

states in this case is found to be seven. The critical values of χ along $\delta = 0$ line are again in agreement with our earlier result [24]. Typical phase diagram of SL states in the (χ, δ) plane with $V = 2$ is also shown in fig.(6). The phase diagram contains one to seven SL states. Furthermore, if we compare the results for $\delta = 0$ with $\delta \neq 0$, we note that maximum number of possible SL states increases as nondegeneracy is introduced.

In passing it is worth to mention that there are $N/2$ stable SL states in a region if the region in the phase plane contain N number of SL states and N is even. On the other hand $(N + 1)/2$ states are stable if N is odd. The stability of a SL state is connected with the variation of the energy of the state as a function of χ . If the energy of the state increases with the increase of χ , the state is stable otherwise unstable. A simpler analysis of stability of a state and its connection with its energy will be presented in the next section.

III. FULLY NON-LINEAR CHAIN WITH ALTERNATIVE NONLINEAR STRENGTHS

Here we consider a fully non-linear 1-dimensional system where the alternative sites are of different strengths. The Hamiltonian of the system is given by

$$H = \frac{1}{\sigma + 2} \sum_{n=-\infty}^{\infty} \chi_n |C_n|^{\sigma+2} + \frac{1}{2} \sum_{n=-\infty}^{\infty} [C_n^* C_{n+1} + h.c.] \quad (13)$$

where ,

$$\begin{aligned} \chi_{2n} &= \chi_1, & -\infty \leq n \leq \infty \\ \chi_{2n+1} &= \chi_2, & -\infty \leq n \leq \infty. \end{aligned} \quad (14)$$

Hopping matrix elements between neighboring sites are taken to be unity. To obtain SL states we consider $C_n = \phi_n e^{-iEt}$ and $\phi_n = \phi_0 \eta^{|n|}$. The expression for η is obtained by taking $|n| \rightarrow \infty$ and is given by $\eta = \frac{1}{2}[|E| - \sqrt{E^2 - 4}]$ [21]. Here we have considered monomeric ansatz because the system is symmetric about the 0-th site. After going through the same procedure as earlier and using the normalization condition , $\phi_0^2 = (1 - \eta^2)/2$, we obtain the reduced Hamiltonian of the dynamical system given by

$$H_{eff} = \frac{1}{\chi(\sigma+2)} \left[\frac{1-\eta^2}{1+\eta^2} \right]^{\frac{\sigma+2}{2}} \left[\chi \frac{1+\eta^{\sigma+2}}{1-\eta^{\sigma+2}} + \delta \frac{1-\eta^{\sigma+2}}{1+\eta^{\sigma+2}} \right] + \frac{2\eta}{1+\eta^2} \quad (15)$$

where χ and δ are defined as $\chi = (\chi_1 + \chi_2)/2$ and $\delta = (\chi_1 - \chi_2)/2$. Setting $\partial H_{eff}/\partial\eta = 0$ we get

$$\frac{1}{\chi} = \frac{(\eta^\sigma - 1)(\eta^{\sigma+4} + 1)}{\left[\frac{\eta^2 - 1}{\eta} \left(\frac{1+\eta^2}{1-\eta^2} \right)^{\frac{\sigma}{2}} - \delta \frac{(\eta^\sigma + 1)(\eta^{\sigma+4} - 1)}{(1+\eta^{\sigma+2})^2} \right] (1 - \eta^{\sigma+2})^2}. \quad (16)$$

Eq.(16) can be used to analyze number of possible states for different values of χ, δ and σ .

For $\sigma = 0$ and $\delta = 0$ from eq.(16) we see that to get a SL state χ needs to be infinite. It, therefore, means that no SL states can be obtained. This is true for $\sigma = 0$ and $\delta = 0$ because the system reduces to a perfect linear system. This is also true for $\sigma = 0$ and $\delta \neq 0$. Analysis of SL states can be done for arbitrary σ but we consider the case of $\sigma = 2$ for the reason mentioned earlier. For $\sigma = 2$, eq.(16) reduces to

$$\frac{1}{\chi} = \frac{\eta(1+\eta^6)(1+\eta^4)^2}{(1+\eta^2)^3[(1-\eta^2)(1+\eta^4)^2 - \delta\eta(1-\eta^2)(1-\eta^6)]} \quad (17)$$

Eq.(17) directly tells that for $\delta = 0$ there will be always one SL state and this is consistent with our earlier result [24]. Using eq.(17) the phase diagram of SL states in (χ, δ) plane is obtained and shown in fig.(7). As usual numbers in different regions indicate number of SL states in those regions. Here also maximum number of SL states increases compared to a perfect nonlinear chain. Furthermore the phase diagram in this case is quite rich (see fig.(7)).

The stability of the SL states in this system can be understood from a simpler graphical analysis. For this purpose we look at the Hamiltonian given in eq.(15). The Hamiltonian is function of one dynamical variable, namely, η where χ and δ are parameters. For fixed values of χ and δ , η and $\partial H_{eff}/\partial\eta = f(\eta)$ can be treated as generalized coordinate and generalized momentum respectively for the reduced dynamical system. Solutions of the equation $f(\eta) = 0$ will give the fixed points for fixed value of χ and δ and number of fixed points with $\eta \in [0, 1]$ will be the number of SL states. We now plot $f(\eta)$ as a function of η for $\chi = 0.35$ and $\delta = 2.5$ as shown in fig.(8). If $f(\eta) > 0$, then the flow of the dynamical

variable will be along the positive direction and on the other hand if $f(\eta) < 0$ the flow will be along the negative direction. These flows are indicated by arrows in the figure and the fixed points are denoted by A, B and C respectively. In the neighborhood of A the flow is always towards A and same for C. Therefore, A and C are stable fixed points. On the other hand in the neighborhood of B the flow is away from B. Hence, this is an unstable fixed point. Same thing happens for all (χ, δ) in the three state region in fig.(7). We therefore notice that among three SL states (fixed points) two are stable and the other one is unstable. To get a connection of the stability of the states with the energy and χ , we plot the energy of the states as a function of χ in the neighborhood of $\chi = 0.35$ for fixed value of $\delta = 2.5$ in fig.(9). Energies of the SL states arising from the fixed points A, B and C are denoted by A_1 , B_1 and C_1 respectively in fig.(9). The figure clearly shows that in the neighborhood of $\chi = 0.35$, the energy of two stable SL states increases with χ and that of the unstable state decreases. We, therefore, conclude that the SL state is stable if the energy of the state increases with χ otherwise unstable.

IV. SUMMARY

We have found the possible number of SL states due to the presence of a quadratic nondegenerate nonlinear dimeric impurity in one dimensional systems. Phase diagram of SL states in (χ, δ) plane is presented for all the systems with a nondegenerate dimeric impurity. Maximum number of SL states is found to increase due to the introduction of nondegeneracy. The dimeric ansatz has been used in this case and this reproduces known results for special cases. A full phase diagram of SL states for a system of one dimensional chain with alternative sites having different nonlinear strength is presented. A monomeric ansatz has been introduced in this case and found to be consistent for special cases. Here also maximum number of SL states increases compared to that in a perfect nonlinear system. A stability analysis for the SL states in the fully nonlinear system and a connection of the stability with the variation of the energy of the state as a function of the nonlinear parameter

are presented.

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FIGURES

FIG. 1. The phase diagram of SL states in (χ, δ) plane for an one dimensional system with a nondegenerate linear dimeric impurity in the middle of the system. The (χ, δ) plane is divided into many regions by the critical lines. The region indicated by 2LA implied the possibility of two SL states in that region and both of them lie above the band of the linear host. Similarly 1LA, 1LB and 2LB implies one SL state above the band, one SL state below the band and two SL states below the band respectively.

FIG. 2. The phase diagram of SL states in (χ, δ) plane for a Cayley tree with a nondegenerate linear dimeric impurity embedded in the middle of the system. The connectivity (K) of the Cayley tree is 4. The region indicated by OL implies that there is no possible SL state in that region. Others are same as in fig. (1).

FIG. 3. The phase diagram of SL states in (χ, δ) plane for one dimensional system with a bond defect ($V = \sqrt{2}$) between sites 0 and 1 as well as a nondegenerate linear dimeric impurity occupying sites 0 and 1. Other things are same as fig. (1) and fig. (2).

FIG. 4. The phase diagram of SL states in (χ, δ) plane for an one dimensional system with a nondegenerate quadratic nonlinear dimeric impurity in the middle of the system. The (χ, δ) plane is divided into many regions by the critical lines. The number in a region indicate the number of possible SL states in the region.

FIG. 5. The phase diagram of SL states in (χ, δ) plane for a Cayley tree with a nondegenerate quadratic nonlinear dimeric impurity embedded in the middle of the system. Here $K = 4$. The number in a region indicates the number of possible SL states in the region. There are two small regions near the origin containing two SL states.

FIG. 6. The phase diagram of SL states in (χ, δ) plane for one dimensional system with a bond defect between sites 0 and 1 as well as a nondegenerate quadratic nonlinear dimeric impurity occupying sites 0 and 1. The bond defect, V is taken to be 2. The number in a region indicates the number of possible SL states in the region.

FIG. 7. Phase diagram of SL states in (χ, δ) plane for a fully nonlinear one dimensional system where alternative sites are of different nonlinear strengths. The number in a region indicates the number of possible SL states in the region.

FIG. 8. $f(\eta)$ is plotted as a function of η . Points indicated by A, B and C are fixed points. Here χ and δ are taken to be 0.35 and 2.5 respectively.

FIG. 9. Energy of SL states are plotted as a function of χ . Here $\delta = 2.5$. A_1, B_1 and C_1 are the points corresponding to the points A, B and C (in fig. (8)) respectively. The dotted line is $\chi = 0.35$.